Demonstration of Capability to Simulate Particle Irregular Shape and Poly-Disperse Mixtures Within Lunar Lander Plume-Surface Interaction

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ABSTRACT

Plume-Surface Interaction (PSI) between lander engine plumes and regolith soil creates hazards in obscuration and contamination by particle clouds, high-energy ejecta streams, and landing area cratering damage. The Gas-Granular Flow Solver (GGFS) enables coupled gas-particle two-phase flow simulations to predict the range of PSI effects from onset of surface erosion to deep crater formation. GGFS features an Eulerian-Eulerian modeling approach, treating both gas and granular material as interacting continuum phases. Eulerian granular material flow modeling requires closure formulations for the granular material constitutive models (stress, friction, collisional and kinetic energy dissipation, drag, etc.). Modeling the lunar regolith granular characteristics poses special challenges due to complex particle shapes and mixture composition. The integration and maturation of the constitutive model database generation process into the GGFS simulation framework are proceeding under funding by the NASA Game Changing Development program. The status of current capabilities in modeling particle shape and mixture effects is presented in comparisons of crater characteristics predicted in Apollo LM plume-surface interaction simulations.

INTRODUCTION

Plume-Surface Interaction (PSI) between lander engine plumes and regolith soil creates hazards in obscuration and contamination by particle clouds, damage by high-energy ejecta streams, and landing area cratering damage. The MSFC Fluid Dynamics Branch is developing simulation tools to offer a predictive PSI capability to NASA customers such as the Human Lander System (HLS) and Commercial Lunar Payload Services (CLPS) [Korzun, 2022; West, 2022; Liever, 2021].

The Gas-Granular Flow Solver (GGFS) was developed for coupled gas-particle two-phase flow simulations to predict the full range of PSI effects from onset of surface erosion to deep crater formation. The GGFS two-phase flow solver features an Eulerian-Eulerian modeling approach, treating both the gas and granular material as continuum phases, to directly compute the interaction of the gas and granular phases at the surface and to simulate erosion, cratering and transport processes. To enable the simulation of gas-particle flows with the Eulerian multi-phase solver, an Eulerian granular phase model was implemented which requires constitutive models (stress,

friction, collisional and kinetic energy dissipation, drag, etc.) for closure of the governing equations. Details of the gas-granular modeling approach and the development of the GGFS simulation tool can be found in [Gale, 2017; Gale 2020].

While closure models for spherical particles can be formulated from particle kinetic theory, closure models for realistic non-spherical particles must be extracted from unit physics Discrete Element Method (DEM) particle interaction simulations and provided in the form of tabular datasets. The effects of particle irregular shape can be simulated by approximating the particle features (non-spherical shape factors, angular particle surface roughness, and interlocking features) in the form of grouped elemental spheres to form composite particles in the DEM simulations. The effects of the wide range of regolith mixture particle sizes and particularly the presence of the small particle sizes results in increased particle interactions and low porosity of the regolith mixture. The range of particle sizes can be simulated by binning the particle sizes into an appropriate finite number of particle-size species and solving the problem as a multi-species mixture. Combining these two modeling approaches enables simulations to capture both, the contributions of the irregular particle shape and the particle size distribution.

Both the DEM based constitutive property database generation and the application of these databases for poly-disperse mixtures have been implemented into the GGFS framework. Full integration and maturation of the DEM-based constitutive model database generation process and poly-disperse mixture binning approach into the GGFS simulation framework are proceeding under funding by the NASA Game Changing Development program [West, 2022; Liever, 2022]. The status of current capabilities is presented in comparisons of crater characteristics resulting for spherical and irregular shape particles, and for mono- and bi-disperse mixture simulations of Apollo Lunar Module plume-surface interaction.

MODELING APPROACH FOR MONO- AND POLY-DISPERSE MIXTURES OF SPHERICAL AND IRREGULAR SHAPED PARTICLES

In the GGFS modeling framework, only a single solid momentum equation and a single granular energy balance are required for a particle mixture combined with N species bin conservation equations. These two equations (momentum and granular energy) require constitutive relations for the dissipation rate of granular energy, the granular energy flux vector, the solid stress tensor, and the mass flux of species which depend on the species number density as well as various transport coefficients (e.g. granular conductivity, pressure, shear and bulk viscosity, etc.). These transport coefficients, in turn, depend on the specific properties of the local particle mixture composition, as well as the flow variables.

Mono-Disperse Spherical

Constitutive relations for spherical particles can be formulated from particle kinetic theory. This is the modeling capability implemented in most gas-particle simulation programs available in academic research or commercial tools. This capability has been integrated in the GGFS framework as the baseline capability.

Poly-Disperse Mixture Formulation (GHD)

To account for the effect of particle size distribution in regolith, the formulation introduced by Garzo, Hrenya & Dufty (GHD) is applied. The GHD formulation extended mono-disperse granular kinetic theory to account for a discrete number of species [Garzo, 2007a; Garzo, 2007b; Murray, 2012a]. Here, a species is a bin of particles of a certain size range. Given the wide particle size distribution of regolith, the challenge is to determine the number of species N in the granular mixture model needed to sufficiently represent the full, continuous distribution. Since the number of governing differential equations increases with increasing number of species - the number that needs to be solved is equal to N + 2 (N species balances, one momentum equation, one granular energy equation) - the computational complexity and cost increases with increasing number of species. Murphy estimated that lunar regolith may be sufficiently represented by a finite (less than 8) number of particle size bins [Murray, 2012b]. For NASA production application efficiency, it will be desirable to limit the number of soil species bins, and thus the number of equations to be solved and the number of soil species DEM database generation runs, to a level that is acceptable for 'engineering accuracy' at various phases of a project.

Discrete GHD Databases Generation and Run-Time Database Interpolation

The GHD model can quickly become computationally too expensive to use on-the-fly in its direct analytical form for large number of species bins representing a poly-disperse composition. The major reasons for this large simulation overhead just from computing mixture coefficients which require the solution of seven linear systems of equations of the size of species number N squared at each computational cell. Since the analytical form of GHD is only suitable for spheres and DEM generated tabular databases will be required for all realistic compositions anyway, the decision was made early during GGFS development to implement a discrete database GHD model featuring adaptive tabular database interpolation methods. A discrete-coefficient algorithm was developed where each of the closure model coefficients is generated as a function of the particle volume fraction and the particle bin mixture fraction state and tabulated prior to the start of a simulation.

The database for a mono-disperse particle results in a one-dimensional database, such as shear stress as a function of volume fraction as shown in Figure 1. For a bi-disperse mixture, the dataset becomes two-dimensional with the volume fraction and the particle bin mixture fraction becoming independent variables, also shown in Figure 1. Whereas the mono-disperse curve in Figure 1 is resolved by eight distinct datapoints in this example, the bi-disperse dataset is discretized with eight volume fraction datapoints and five mixture fraction datapoints, with s=0 being all irregular particles and s=1.0 being all spheres. Thus, the dataset now has two independent parameters and requires a two-dimensional interpolation. For poly-disperse mixtures with N greater than two, the size of the database discrete point goes up by the datapoints to the power of N and an N-dimensional search and interpolation algorithm is required.

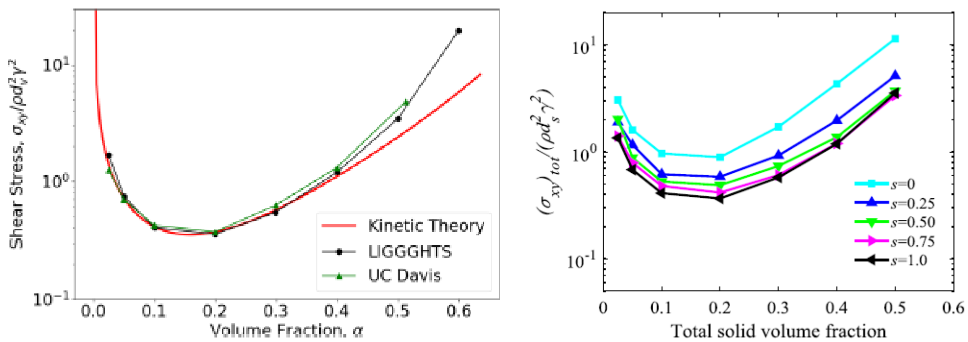
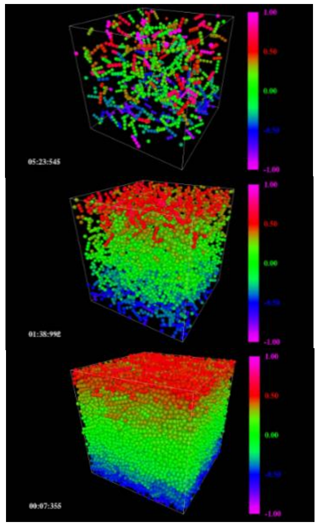


Figure 1. Total Shear Stress as a function of Solid Phase Volume Fraction Ratio. Left: Mono-disperse sphere; Right: Bi-disperse

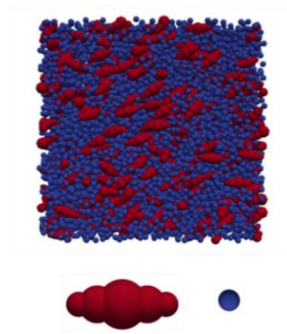
The initial implementation of the discrete GHD model implementation was performed for a bi-disperse mixture since two-dimensional, computationally efficient database interpolation algorithms were readily available in the Loci computational framework the GGFS is implemented in. Loci offered efficient, two-dimensional, adaptive, tabular representations for complex equations of state required in reacting flow and phase change modeling. A general N-dimensional interpolation module for N-dimensional database interpolations was initially not available in the Loci computational framework. The required N-dimensional interpolation capability in the Loci framework has now been implemented by the developers of the Loci framework and is currently being integrated by the GGFS development team. This is the crucial step in extending the mixture simulation capability from current bi-disperse to a general number of size bins.

Irregular Shape – DEM Database Generation

Closure models for realistic non-spherical particles must be extracted from unit physics Discrete Element Method (DEM) particle-particle interaction simulations and provided in the form of tabular datasets. The effects of particle irregular shape (non-spherical shape factors, angular particle surface roughness, and interlocking features) are simulated by approximating the particle features in the form of grouped elemental spheres to form composite particles in the DEM simulations. Figure 2 shows examples of DEM simulations for spherical and irregular shapes, as well as mixtures of different shapes in a poly-disperse mixture analysis [Guo, 2012; Guo, 2013; Guo, 2015; Yang, 2019]. While database generation for a variety of particle shapes have been demonstrated, only cylinder shaped particle DEM-based databases were implemented during the initial GGFS framework prototype implementation to verify and mature the irregular shape capability. At this point in the GGFS development cycle, the GGFS framework provides operational capabilities for mono-disperse cylindrical particles with aspect ratios of h/d = 1, 2, 4, 6.



Glued-sphere approximation of irregular particle shape



DEM simulations capturing particle volume fractions effects

DEM simulation of bi-disperse mixture of spherical and composite irregular shape

Figure 2. DEM simulation examples [Guo, 2012, 2013, 2015; Yang, 2019]

The end target has always been the on-demand generation of a database for any user defined particle shape. The irregular shaped particle DEM simulation and Eulerian constitutive database generation processes in the initial development of the GGFS framework were performed with research-oriented DEM tools developed by academic partners. Assessment of the computational efficiency and practicality of the academic serially executed DEM tools on NASA supercomputers identified the need to migrate to a DEM framework capable of performing parallel simulations on NASA supercomputer assets in a process orchestrated in an automated setup, execution, database extraction, and dataset delivery ready for application simulations. The LIGGGHTS DEM toolset has been selected as the most suitable tool to migrate the DEM simulations. Extension to rapid, production oriented on-demand database generation for user specified particle shapes is now within reach pending efficient implementation of a streamlined DEM database generation procedure [Howison, 2022].

Combining these modeling approaches enables simulations to capture both, the contributions of the irregular particle shape and the particle size distribution. The integration and maturation of the DEM-based constitutive model database generation process and poly-disperse mixture binning approach into the GGFS simulation framework are proceeding under funding by the NASA Game Changing Development program.

DEMONSTRATION OF CURRENT MODELING CAPABILITIES: APOLLO LUNAR MODULE PLUME INDUCED CRATERING

This paper presents the evaluation of GGFS predictive capabilities during the FY2021 of the multi-year PSI project. The purpose was two-fold: to evaluate Loci/GGFS performance for plume flow simulations in near vacuum conditions, and to evaluate the available modeling for realistic particle shape and mixture effects.

A demonstration of the current capabilities was performed for a 3D cratering simulation of Apollo LM at an altitude of 5 meter of the nozzle exit above the Lunar surface. The LM nozzle has an exit diameter of 1.457m. By simulating cratering from Apollo LM, current capabilities for a set of realistic conditions can be assessed with respect to a representative human lander landing on the Moon. The Loci/GGFS tool is used to simulate the 3D geometry shown in Fig. 3 below. The domain has a radial extend of 25m and a total height of 25m. A regolith layer 3m deep below the surface is comprised of particle mixtures of the four compositions evaluated.

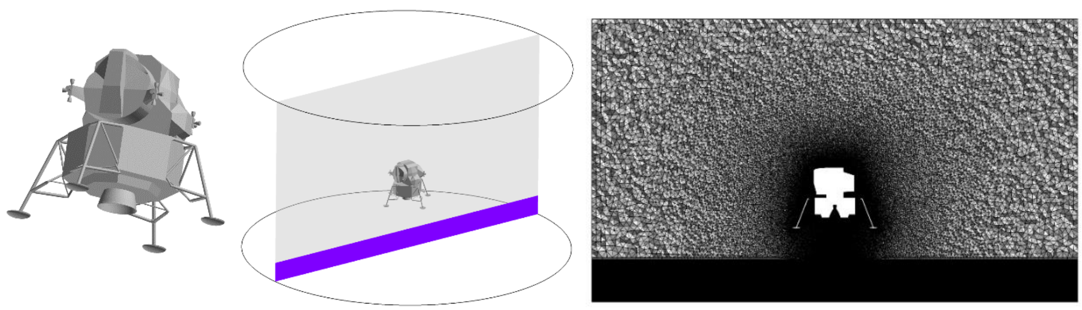


Figure 3: Computational geometry of for Apollo LM crater formation simulation for nozzle exit at 5m elevation above a 3m deep soil layer.

At this point in the GGFS development cycle, the framework had operational capabilities for mono-disperse spherical and for cylindrical particles, and the ability to perform bi-disperse mixtures of spherical particles using the GHD tabular database approach. Lunar plume cratering simulations were therefore performed for mono-disperse spheres with 30 micron and 100 micron diameters, a bi-disperse mixture of the 30mi+100mi spheres with a solid volume fraction of 50% for each, and a mono-disperse cylindrical particle with an aspect ratio of AR=4. The particles are shown in Figure 5. These particle variations allowed the check-out of GGFS for all available options and assessment of the effects of the variations in shape and mixture and the operational maturity status of those modeling options.

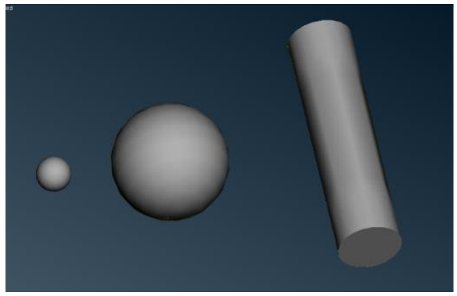


Figure 5. Particle shapes and sizes evaluated: 30-micron sphere, 100-micron sphere, aspect ratio AR=4 cylinder with volume equivalent to 100-micron sphere

Lunar regolith was modeled with a density of 3,000 kg/m^3 assuming solid particles with no internal voids or porosity. A linear elastic solid model was applied with internal friction angle of 45 degrees and a particle collision coefficient of restitution of 0.95.

The simulation is performed with the entire domain set to an initial ambient pressure of 0.1 Pa, a relatively low but non-zero pressure to demonstrates the ability of the currently continuum-only solver to perform in the vacuum environment on the Moon. Extension of the GGFS capabilities to mixed continuum-rarefied flow physics is in early development. The plume flow is composed of a Hydrazine combustion product surrogate gas and initiated from the engine chamber inflow conditions at 23 psi chamber pressure. This corresponds to Apollo LM terminal descent thrust levels of approximately 2200 lbf. The plume flow is initiated impulsively through the nozzle into the initial quiescent domain and impinges on the regolith surface to quickly progress into a fully developed plume flow field. At the low elevation of 5m, the plume flow expands to a supersonic outflow in both outward and upward directions, as shown in Figure 4. Note how the plume flow escapes from the stagnation region forming inside the developing crater in an outward supersonic, high shear flow pattern along the crater walls and the lunar surface as the main erosion mechanism.

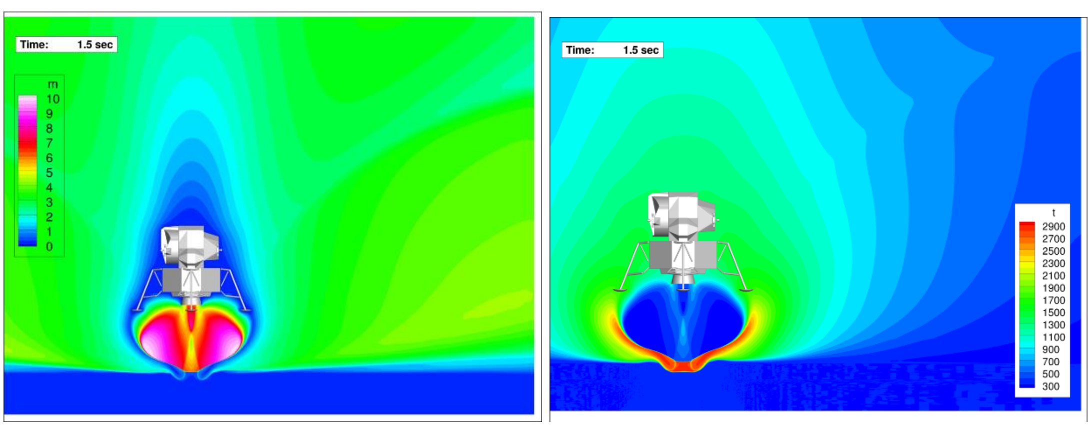


Figure 4: Flowfield details of Apollo LM crater formation simulation for 5m nozzle exit elevation. Left: Mach number; Right: Gas Temperature

The resulting particle ejecta patterns can be observed from contours of solid phase volume fraction at the log10 scale shown in Figure 6 for the simulations with 100-

micron sphere particles. As the plume initially impinges on the lunar surface below, regolith is lofted and ascends upward with the farfield plume flow. Once the quasi-steady plume field has settled, ejecta sheets form at radial locations slightly outboard under the plume expansion region. The ejecta streams escape radially outwards at low angles in the 5 to 10 degree range. This ejecta pattern compares well to those observed in actual landing footing.

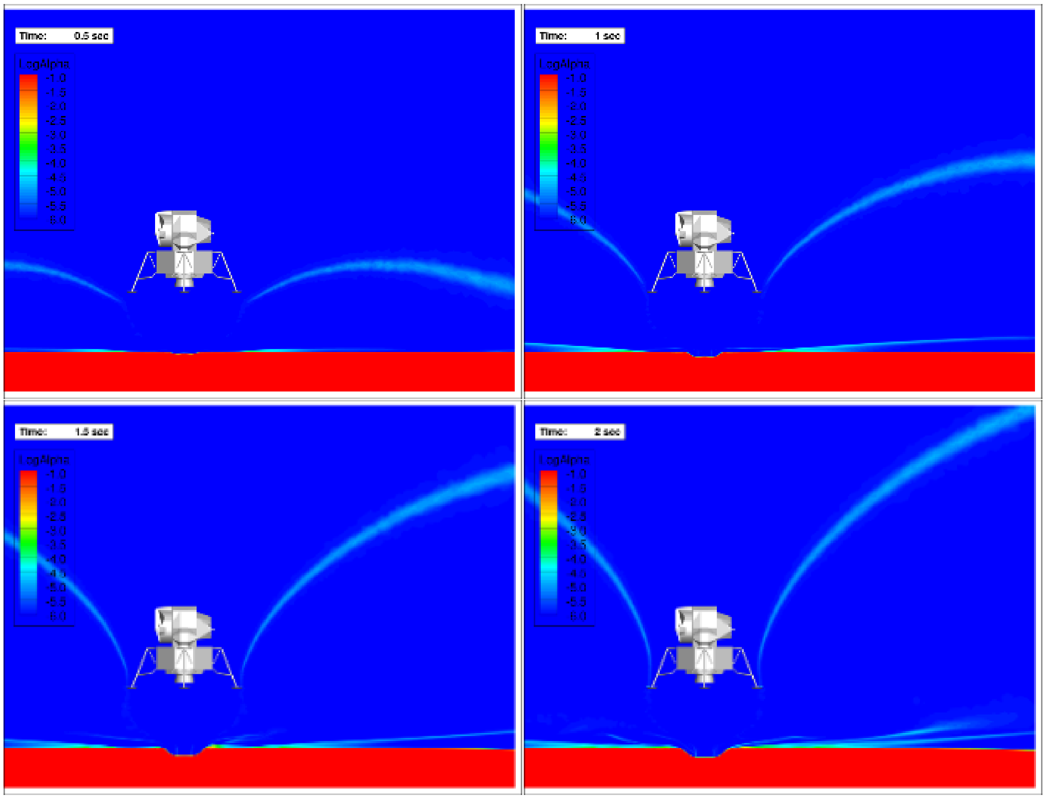


Figure 6: Contours of solid phase volume fraction (log10) for 100-micron mono-disperse sphere particles indicating evolution of crater and shallow angle near-surface ejecta sheets, with ascending particle cloud resulting from impulsive plume start-up

A total of two seconds of flow time was simulated, resulting in a relatively wide but shallow crater of approximately 0.75m depth and diameter approaching 4.0m, as shown in Figure 7 below, again for the 100-micron sphere particles. Such crater dimensions are obviously much larger than actual craters observed for the actual lunar regolith composition. The crater side walls display local lobe and pocket features which indicates that while the gross crater shape is circular, the local gas-particle interaction occurs in a three-dimensional, multi-modal pattern.

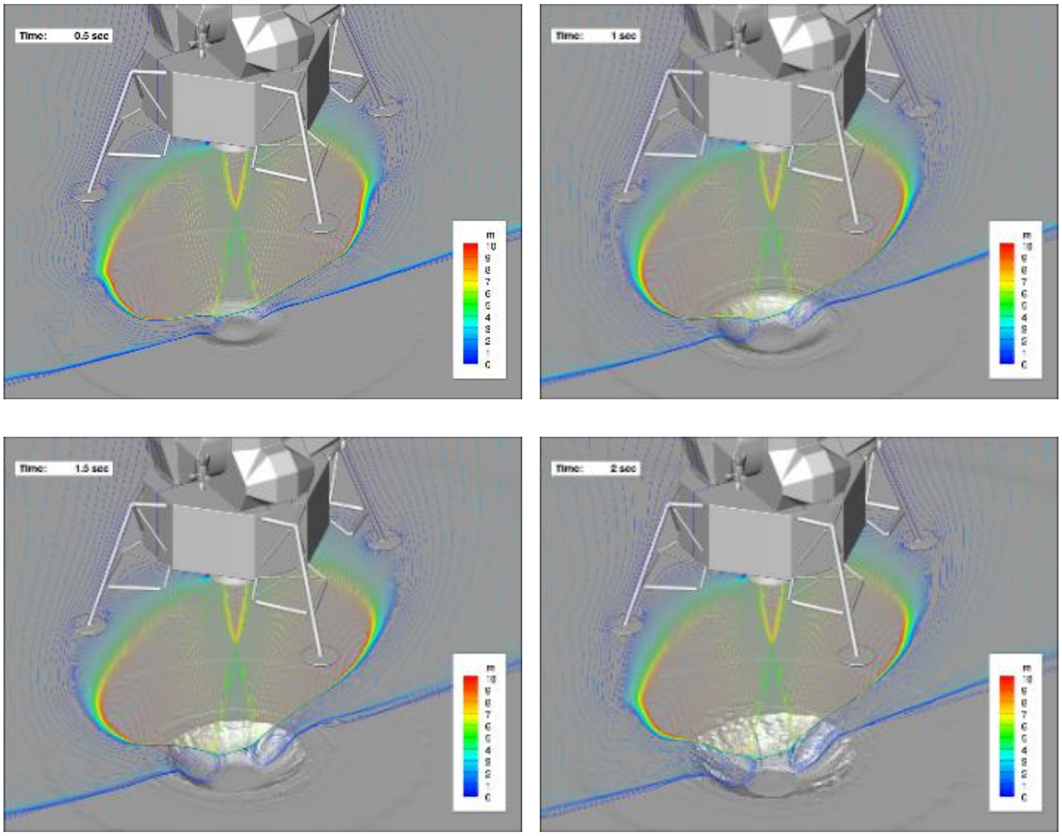
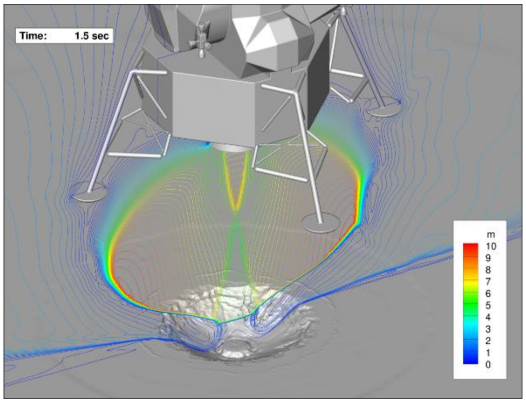
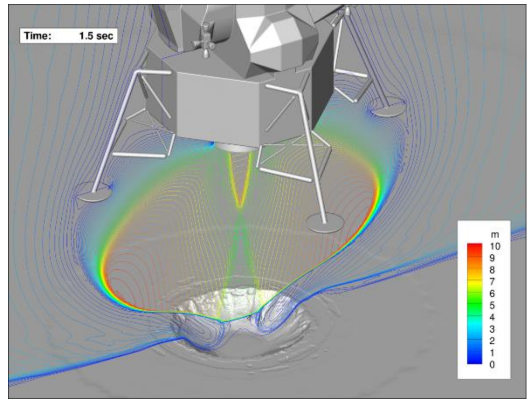


Figure 7: Progression of crater shape for 100-micron mono-disperse spheres at half-second intervals up to two seconds

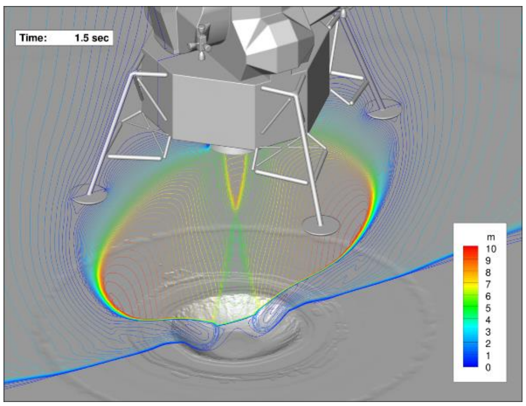
Figure 8 compares the crater shape size and local features for the four compositions modeled at t=1.5sec of simulation time. The crater walls show more pocketed appearance for small spheres compared to the larger spheres. The non-spherical elongated shape (cylinder AR=4) results in reduced crater depth compared to spheres. Bi-disperse mixture results in highest reduction in crater depth and a much shallower crater. Thus, both the size, the shape and the bi-dispersity of the particles result in distinctly different resulting crater features.



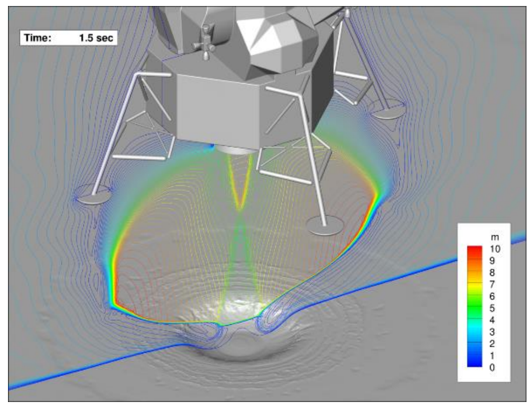
Spheres 30 micron



Spheres 100 micron



Cylinder AR=4



Bi-disperse Spheres 30+100 micron

Figure 8: Crater shapes at t=1.5 seconds for four composition modeled

Figure 9 shows the cross-sections of the craters at simulation time t=1.5sec. The smaller 30-micron spheres form an erosion trough in the outer region of crater floor, with a distinct plateau remaining under the central post-normal shock region. The non-spherical irregular elongated shape (cylinder AR=4) results in reduced crater depth compared to spheres. The bi-disperse mixture (30micron+100micron) results in even more reduced crater depth. Thus, even the first step from mono- to bi-dispersity shows a sizable reduction in erosion strength and crater size.

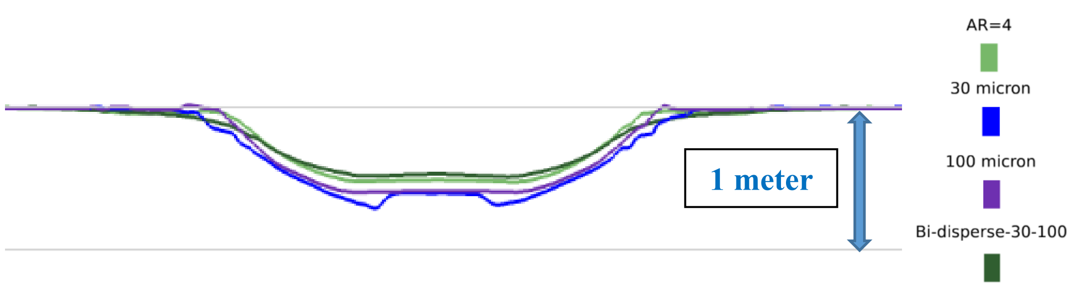


Figure 9: Cross section profiles at t=1.5 seconds for four compositions modeled.

At the submission of this paper, additional simulations are performed with the tri-disperse sphere analytical GHD model to extend the poly-disperse effects to a tri-disperse level. A prototype of the multi-dimensional discrete GHD interpolation methodology is being integrated and general N-disperse modeling capability will be tested beyond the bi- and tri-disperse mixture level. This capability will provide considerable progress in simulation capability and insight into the significance of wider resolution of the particle size in a mixture. Results will be published during the 2022 year of the PSI project.

CONCLUSION

The application readiness of the soil models currently operational in GGFS was presented for the example of a full scale, 3-D simulation of the plume induced erosion and crater formation of the Apollo LM at an elevation of 5m above ground in a low pressure, near vacuum background. Comparison of the predicted crater shape differences between soil models with spheres, irregular cylindrical particles, and a bi-disperse sphere mixture confirmed the significance of the irregular shape and mixture effects. The current modeling capabilities will be extended towards rapid on-demand DEM based particle database generation and efficient database access during simulations for larger numbers of mixture bins. Application testing and validation of these capabilities will be performed against experimental data generated under the GCD PSI project.

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